PROJECT NUMBER: 1754
PROJECT TITLE: Spectroscopic Studies of Tobacco and Smoke Components
PROJECT LEADER: J. B. Wooten
PERIOD COVERED: October, 1987

I. SOLID STATE NMR

A. Objective: Characterize tobacco and related products by ^{13}C CP/MAS NMR.

B. Results: Two Japanese RL products were examined by solid state NMR for the presence of higher than average levels of cellulose. The C-4 signal of cellulose is free from interfering signals in intact and composite plant materials. The intensity of this signal can be used to make a crude estimate of the relative amount of cellulose present. Both Japanese RL products exhibit enhanced signals for C-4 at 89 ppm relative to Philip Morris RL. One sample contains at least twice the PM level of cellulose. This same sample exhibits an unusual carboxyl region signal at 179 ppm which is not typical of either intact plant or composite plant materials. Carboxymethyl cellulose, which is commonly used as a binder, exhibits a strong carboxyl signal at 178 ppm, and is being investigated as the possible source of this unusual signal.

A. Objective: Determine the local environment and mobility of nicotine in tobacco in situ.

B. Results: A detailed, technical memo describing the use of isotopic labeling and solid state NMR for the the detection of nicotine in tobacco was recently issued.

C. Reference:

Memo from J. Wooten to R. Izac, "In Situ Detection of Nicotine in Tobacco by ^{13}C CP/MAS NMR", October 21, 1987.

II. SOLUTION NMR

A. Objective: Determine the degree of esterification of degraded pectins.

B. Results: We are currently using ^{13}C solution NMR to determine the per cent of methyl esterification in degraded pectin samples submitted by Sherry Baldwin. The degree of esterification is obtained by integrating the carboxyl region signals which exhibits well resolved signals for the esterified and free carboxyl groups. The NMR results compare favorably with those obtained by the titration method. The availability of different pectin samples that have been degraded to varying extent affords the opportunity to look for differences in their ^{13}C spectra that might result from the variation in the polymer chain length. At least five distinct spectral patterns have been identified for different pectin samples in the region between 95 and 110 ppm that contains the anomeric

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carbon signals. As many as five, or as few as two groups of signals appear in the spectra of different samples. These differences may be useful for characterizing the extent of degradation in pectin being prepared for use as a foamed binder.

C. **Plans**: The signals in the anomeric region of the degraded pectins will be identified and correlated with pectin structure.

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